

# Thread bonds in molecules

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Unusual chemical bonds are proposed. Each bond is almost covalent but is characterized by the thread of a small radius,  $\sim 0.6 \times 10^{-11}$  cm, between two nuclei in a molecule. The main electron density is concentrated outside the thread as in a covalent bond. The thread is formed by the electron wave function which has a tendency to be singular on it. The singularity along the thread is cut off by electron “vibrations” due to the interaction with zero point electromagnetic oscillations. The electron energy has its typical value of  $(1 - 10)$  eV. Due to the small thread radius the uncertainty of the electron momentum inside the thread is large resulting in a large electron kinetic energy  $\sim 1$  MeV. This energy is compensated by formation of a potential well due to the reduction of the energy of electromagnetic zero point oscillations. This is similar to formation of a negative van der Waals potential. Thread bonds are stable and cannot be created or destructed in chemical or optical processes.

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## I. INTRODUCTION

Various types of chemical bonds in molecules are well studied. See for example [1–3]. This is a branch of chemical physics with the well established set of basic phenomena. Methods of quantum chemistry are effectively applied to develop that field. The common feature of chemical bonding is the typical energy. Despite a variety of bond types there is the upper limit of energies involved into the phenomena. It is the atomic scale energy of the order of ten electron volts. Also the typical spatial scale in chemical bonding is no shorter than the atomic size.

It looks unusual if energies, involved into molecular bonding, are of the order of 1 MeV and the spatial scale is  $10^{-3}$  of the size of hydrogen atom. At the first sight, it is impossible since chemical bonding is associated with the atomic processes.

The point is that the electron state can have a tendency to be singular along the line (thread) connecting two nuclei in a molecule. The origin of such singularity is clear from Schrödinger equation in cylindrical coordinates which can have the solution logarithmically singular on the axis. The electron “vibrates” due to the interaction with zero point electromagnetic oscillations and the singularity smears out within the thread of a small radius  $0.6 \times 10^{-11}$  cm. This radius can be determined accounting for electron-photon interaction in quantum electrodynamics since due to short scales the electron momentum becomes relativistic.

The exact state, where the electron is coupled to photons, is steady and is characterized by the certain total energy which is conserved. In terms of Schrödinger equation it would be an energy eigenvalue. The state, considered either far from the thread or inside it, corresponds to the same energy. The large contribution to the electron kinetic energy  $\sqrt{(mc^2)^2 + (\hbar c/r_T)^2} - mc^2 \simeq 2.93$  MeV inside the thread should be compensated by a reduction of the electromagnetic energy. The latter can be roughly

interpreted as a potential well at the thread region. One can say that the thread state with the chemical electron energy  $(1 - 10)$  eV corresponds to upper energy states in the deep potential well, of the order of 1 MeV, and of the radius  $0.6 \times 10^{-11}$  cm. This well is extended along the thread. The electron number is determined by the outer region with respect to the thread. This region is of the order of the Bohr radius as in a covalent bond.

This is not the unique situation of application of quantum electrodynamics in chemistry. The famous example is van der Waals forces when quantum electrodynamics is involved. In that case the certain attraction potential is also formed due to the reduction of the energy of electromagnetic zero point oscillations.

The high energy parts, involved into thread formation, correspond to the typical time  $10^{-22}$  s. Optical processes are slow compared to that time. They lead to an adiabatic motion of the thread parameters but absorption probability of such quanta is exponentially small. The life time of the thread bond itself is exponentially large (practically infinity) until a high energy particle or  $\gamma$ -quantum destroys it. Also the thread bond cannot be created in chemical or optical processes. The above high energy impact is necessary for that.

Thread bonds can be created by an external high energy radiation. One can put a question on a role of such stable bonding in biological processes.

In section II the singular (between two Coulomb centers) solution of Schrödinger equation is obtained. In section III the inner thread properties are studied.

## II. MODEL WITH TWO COULOMB CENTERS

Electrons wave function in a molecule is complicated. The electron motion is collective and is not reduced to a single electron problem. The electron wave function is smooth in the space. We focus on the certain speci-

ficity of this function. If to consider usual atomic sizes the electron wave function can be formally singular on some line connecting two nuclei in the molecule. In the exact wave function the singularity is cut off at distances shorter than atomic ones.

Therefore the problem is separated in two parts. First one should find the singular solution of quantum mechanical equations for electrons in the molecule. Second one should analyze mechanisms of smearing of that singularity. In this section we focus on the singularity formation on the line connecting two nuclei which can be treated in the molecule as static ones according to the Born-Oppenheimer approximation.

Instead of solving the problem in full one can simplify it considering a single electron. The main features of the singular wave function can be demonstrated studying the artificial situation when one electron is in the field of two positive charges fixed at two points. The singularity line, connecting two nuclei in the molecule, is associated with large energies and is hardly influenced by chemical forces. For this reason the singularity line between two real nuclei in the molecule is of the same type as between two point charges formally fixed in the space.

### A. Formalism

To study the electron in the Coulomb field of two positive point charges at the points  $z = \pm\sigma$  it is convenient, instead of cylindrical coordinates  $r = \sqrt{x^2 + y^2}$ ,  $z$ , and  $\varphi$ , to use the elliptic ones  $\xi$ ,  $\eta$ , and  $\varphi$  [4]

$$\xi, \eta = \frac{r_2 \pm r_1}{2\sigma}. \quad (1)$$

Here  $r_{1,2} = \sqrt{(z \mp \sigma)^2 + r^2}$  are distances to the Coulomb centers shown in Fig. 1. The surface of a constant  $\xi$  is the ellipsoid

$$\frac{z^2}{\sigma^2 \xi^2} + \frac{r^2}{\sigma^2 (\xi^2 - 1)} = 1 \quad (2)$$

with the focuses at  $z = \pm\sigma$ . The surface of a constant  $\eta$  is the hyperboloid

$$\frac{z^2}{\sigma^2 \eta^2} - \frac{r^2}{\sigma^2 (1 - \eta^2)} = 1 \quad (3)$$

with the focuses at the same points. The coordinate  $\xi$  takes values from 1 to  $\infty$  and  $\eta$  from  $-1$  to  $1$ . Intersections of the surfaces (2) and (3) with the plane  $y = 0$  are shown in Fig. 1.

The Coulomb interaction potential is

$$U = -\frac{Ze^2}{r_1} - \frac{Ze^2}{r_2} = -\frac{2Ze^2}{\sigma} \frac{\xi}{\xi^2 - \eta^2}, \quad (4)$$

where  $Ze$  is the positive charge at each center. The Schrödinger equation for the electron

$$-\frac{\hbar^2}{2m} \nabla^2 \psi + U\psi = E\psi \quad (5)$$

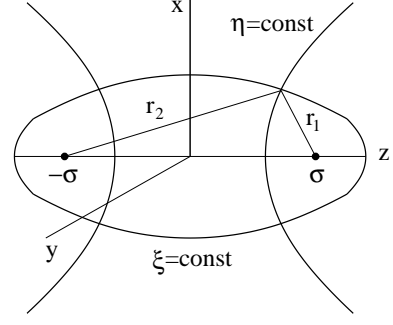


FIG. 1: Intersections of surfaces of constant elliptic coordinates  $\xi$  and  $\eta$  with the plane  $y = 0$  are shown. Two Coulomb centers are at the points  $z = \pm\sigma$ .

in elliptic coordinates takes the form

$$-\frac{\hbar^2}{2m\sigma^2(\xi^2 - \eta^2)} \left[ \frac{\partial}{\partial \xi}(\xi^2 - 1) \frac{\partial \psi}{\partial \xi} + \frac{\partial}{\partial \eta}(1 - \eta^2) \frac{\partial \psi}{\partial \eta} \right] - \frac{2Ze^2}{\sigma} \frac{\xi}{\xi^2 - \eta^2} \psi = E\psi. \quad (6)$$

We consider an axially symmetric wave function. Since the variables are separated it has the form  $\psi(\xi, \eta) = \psi_1(\xi)\psi_2(\eta)$ . One can introduce dimensionless parameters  $\varepsilon = -2m\sigma^2 E/\hbar^2$  and  $p = 4Z\sigma/r_B$  where  $r_B = \hbar^2/(me^2)$  is the Bohr radius.

After separation of variables the two Schrödinger equations are

$$-\frac{\partial}{\partial \xi}(\xi^2 - 1) \frac{\partial \psi_1}{\partial \xi} = (p\xi + \beta - \varepsilon\xi^2)\psi_1 \quad (7)$$

$$-\frac{\partial}{\partial \eta}(1 - \eta^2) \frac{\partial \psi_2}{\partial \eta} = (\varepsilon\eta^2 - \beta)\psi_2, \quad (8)$$

where  $\beta$  is some constant.

The variable  $\eta$  can be written as  $\eta = \cos \chi$ . Then Eq. (8) has the form

$$\frac{1}{\sin \chi} \frac{\partial}{\partial \chi} \left( \sin \chi \frac{\partial \psi_2}{\partial \chi} \right) = (\beta - \varepsilon \cos^2 \chi) \psi_2. \quad (9)$$

The solution, non-singular at  $\chi = 0$ , should be also non-singular after continuation to  $\chi = \pi$ . This is the condition to choose the parameter  $\beta$  for a given  $\varepsilon$ . When two Coulomb centers coincide ( $\sigma = 0$  and therefore  $\varepsilon = 0$ ) that condition turns to  $\beta = -l(l+1)$  as for Legendre polynomials [5]. In that case the variable  $\chi$  coincides with the azimuthal angle  $\theta$ .

### B. Close Coulomb centers

Below two close Coulomb centers are considered under the condition  $\sigma \ll r_B$ . We study the state which is isotropic ( $l = 0$ ) in the limit  $\sigma = 0$ . At a finite  $\sigma$  there is

the small correction to the wave function which can be written as  $\psi_2 = 1 + \delta\psi_2$ . Using the relation

$$\sin \chi \frac{\partial \delta\psi_2}{\partial \chi} = \int d\chi (\beta - \varepsilon \cos^2 \chi) \sin \chi \quad (10)$$

one can obtain

$$\delta\psi_2 = \left(\frac{\varepsilon}{3} - \beta\right) \ln \left(2 \cos^2 \frac{\chi}{2}\right) - \frac{\varepsilon}{6} \sin^2 \chi. \quad (11)$$

The solution (11) is finite at  $\chi = 0$  ( $\eta = 1$ ). In order to get it finite at  $\chi = \pi$  ( $\eta = -1$ ) it should be  $\beta = \varepsilon/3$ . Note that  $\varepsilon \sim p^2 \sim \sigma^2/r_B^2$  are small.

At  $\sigma \ll r_B$  there is a small region of the size  $\sigma$  around the centers in Fig. 1. This region corresponds to  $\xi \sim \eta \sim 1$ . The region of the order of the Bohr radius  $r_B$  is much larger and relates to large  $\xi$ . We consider first this region. In Eq. (7) one can omit  $\beta$  and to write  $\xi^2 - 1 \simeq \xi^2$ . In the limit  $1 \ll \xi$  Eq. (7) takes the form

$$-\frac{\partial^2 \psi_1}{\partial \xi^2} - \frac{2}{\xi} \frac{\partial \psi_1}{\partial \xi} - \frac{p}{\xi} \psi_1 = -\varepsilon \psi_1, \quad (12)$$

which coincides with the radial Schrödinger equation with  $l = 0$  in the Coulomb field of the point charge  $2Ze$  [5]. The solution of (12), decaying on infinity and finite at small distances, corresponds to the eigenvalue  $\varepsilon = p^2/4$ . This value relates to the ground state energy in the Coulomb field of the point charge  $2Ze$ .

For our purposes one needs a solution which also decays on infinity but is singular at  $r = 0$  and  $z^2 < \sigma^2$ . To obtain that one should write the solution of (12) in the form [5]

$$\psi_1(\xi) = \xi^{p/(2\sqrt{\varepsilon})-1} \exp(-\xi\sqrt{\varepsilon}) \times G\left(1 - \frac{p}{2\sqrt{\varepsilon}}, -\frac{p}{2\sqrt{\varepsilon}}, -2\xi\sqrt{\varepsilon}\right), \quad (13)$$

where

$$G(\alpha, \beta, v) = 1 + \frac{\alpha\beta}{1!v} + \frac{\alpha(\alpha+1)\beta(\beta+1)}{2!v^2} + \dots \quad (14)$$

To obtain the solution at shorter distances one should use the asymptotics of the function (14) at  $v \ll 1$ . Thus at small  $[1 - p/(2\sqrt{\varepsilon})]$  one can obtain from Eq. (13) [5]

$$\psi_1(\xi) = 1 + \left(1 - \frac{p}{2\sqrt{\varepsilon}}\right) \frac{1}{2\xi\sqrt{\varepsilon}}, \quad 1 \ll \xi \ll r_B/\sigma. \quad (15)$$

On the other hand, at not large  $\xi$  the left-hand side of Eq. (7) is the principal one and the solution is

$$\psi_1(\xi) = 1 + \frac{1}{4\sqrt{\varepsilon}} \left(1 - \frac{p}{2\sqrt{\varepsilon}}\right) \ln \frac{\xi+1}{\xi-1}, \quad 1 < \xi \ll r_B/\sigma. \quad (16)$$

Eq. (16) goes over into the form (15) when their applicability intervals overlap.

The wave function along the line, connecting two Coulomb centers in Fig. 1, now can be written at  $|z^2 - \sigma^2|, r^2 \ll \sigma^2$  in the form

$$\psi(r, z) = 1 - \frac{r_B}{16Z\sigma} \left(1 - \frac{E}{E_0}\right) \times \ln \frac{8\sigma^2}{z^2 - \sigma^2 + \sqrt{(z^2 - \sigma^2)^2 + 4\sigma^2 r^2}}, \quad (17)$$

where  $E_0 = -m(2Ze^2)^2/(2\hbar^2)$ . Eq. (17) is also valid in the vicinity ( $r^2 \ll (\sigma^2 - z^2)$ ) of the entire line ( $z^2 < \sigma^2$ ) between the centers, where

$$\psi(r, z) = 1 - \frac{r_B}{8Z\sigma} \left(1 - \frac{E}{E_0}\right) \ln \frac{2\sqrt{\sigma^2 - z^2}}{r}. \quad (18)$$

At large distances, as follows from (13) - (14) and the definition (1),

$$\psi(r, z) = R^{\sqrt{E/E_0}-1} \exp\left(-R \frac{2Z}{r_B} \sqrt{\frac{E}{E_0}}\right), \quad r_B \ll R, \quad (19)$$

where  $R^2 = r^2 + z^2$ .

The wave function of the electron in the Coulomb field of two positive point charges  $Ze$  exponentially decays at large distances (19). But on the line, connecting two charges,  $\psi$  has the logarithmic singularity (18) if the energy does not coincide with the eigenvalue  $E_0$ . The absence of singularities is a usual condition to determine an eigenvalue. The eigenvalue  $E_0$  coincides with one in the Coulomb field of one point charge  $2Ze$ . In the limit considered,  $\sigma \ll r_B$ , corrections to that eigenvalue are small.  $E_0$  is the lowest energy level shown in Fig. 2(b) where the potential energy (4) relates to the curve with the dashed insert. The eigenfunction is plotted in Fig. 2(a) with the dashed part of the curve.

When the energy differs from  $E_0$  the singular wave function is not physical at the first sight. But the situation is more complicated as described in Sec. III.

### III. ELECTRON THREADS

The electron wave function, for the artificial case of two static point charges, and the wave function for two partner nuclei in a real molecule have common properties. This happens since at short distances (less than  $r_B$ ) atomic forces are not significant. In the real molecule close to a nucleus, that is below the shell of inner electrons, the wave function is of the type (17). The same is valid for the nucleus at a partner site. Between the partner sites the wave function is logarithmically singular, as (18), along the connecting line  $-\sigma < z < \sigma$ . In a real molecule  $\sigma \sim r_B$ . In a close vicinity ( $r \ll \sigma$ ) of the line, connecting two partner sites, the wave function, with the

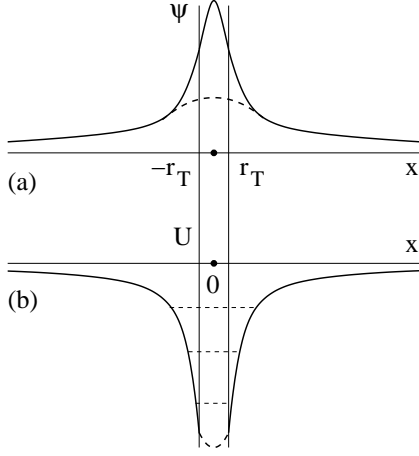


FIG. 2: Features of the thread state at  $y = 0$  and constant  $\eta$ . Dashed curves correspond to the absence of tread. Thin vertical lines restrict the thread region. (a) Thread wave function. (b) Energy levels in the potential well in the absence of thread.

logarithmic accuracy, can be written in the form

$$\psi = \begin{cases} A(\sigma) \ln[\sqrt{(z-\sigma)^2 + r^2} + (z-\sigma)], & |z-\sigma| \ll \sigma \\ 2A(z) \ln r, & \sqrt{\sigma^2 - z^2} \sim \sigma \\ A(-\sigma) \ln[\sqrt{(z+\sigma)^2 + r^2} - (z+\sigma)], & |z+\sigma| \ll \sigma \end{cases} \quad (20)$$

Here  $A(z)$  is the certain function accounting for real intramolecular forces. The exact form of this function is not crucial for our purposes.

An electron, acted by an external macroscopic field, is spatially smeared due to the interaction with zero point electromagnetic oscillations [6]. If  $\vec{u}$  is the electron displacement from its mean field position then  $\langle \vec{u} \rangle = 0$  and  $r_T = \sqrt{\langle u^2 \rangle}$  is finite. In an external field (for example Coulomb one) due to the uncertainty in electron positions it probes various parts of the potential. This changes its energy. The famous example of this phenomenon is the Lamb shift of atomic levels [6].

The electron momentum is not conserved in virtual processes and the electron “vibrates”. The uncertainty  $r_T$  results in small corrections (such as Lamb shift) when the spatial scale of the electron wave function is larger than  $r_T$ . But when the wave function, as a solution of quantum mechanical equations, has a singularity that uncertainty plays a significant role resulting in smearing of the singularity within  $r_T$ .

Therefore the singularity line between two nuclei in a molecule has the finite width of the order of  $r_T$ . It can be called *thread bond*. In Fig. 2(a) the wave function increases towards the tread and it is cut off on the thread size  $r_T$ . The potential energy in Fig. 2(b) is of the usual Coulomb type outside the thread region. Inside the thread the mean field potential no more exists because photon degrees of freedom enter the game.

The singularity of the wave function is cut off on the distance  $r_T$  and the state becomes physical. So

the expression (20) corresponds to not small distances  $r^2, |\sigma^2 - z^2|$ . According to Eqs. (17) and (18), the singular solution of the Schrödinger equation exists at any pre-logarithmic factor  $(1 - E/E_0)$ . This means that the electron energy of the thread state is not quantized due to the interaction with photons. This can be explained in another way. Broadening of discrete levels in a well (quasi-continuous density of states) is narrow and can be calculated from the perturbation theory. Calculation of smearing of the singular wave function requires all orders of the perturbation theory. In this case the density of states is smoothly continuous.

### A. Estimate of the thread radius

Unlike the Lamb shift, it is impossible to apply the perturbation theory to calculate smearing of a singular wave function of electron. In that problem one should account for all orders of the perturbation theory. For this reason, we use below the approximate method just to estimate the electron mean squared displacement [7]. The method is successfully applied for study of the Lamb shift. In this method the electron motion under the action of zero point oscillations can be described by the equation

$$m \frac{d^2 \vec{u}}{dt^2} + m \Omega^2 \vec{u} = -e \vec{\mathcal{E}}, \quad (21)$$

where  $m$  is the electron mass and  $\Omega \sim m e^4 / \hbar^3$  is the electron rotation frequency in the atom.

One can use the Fourier expansion

$$\vec{u}(\vec{R}, t) = \sum_k \vec{u}_k \exp(i \vec{k} \vec{R} - i \omega_k t) \quad (22)$$

and analogous one for the fluctuating electric field  $\vec{\mathcal{E}}(\vec{R}, t)$ . Since  $\vec{u}(\vec{R}, t)$  is real it should be  $\vec{u}_k^* = \vec{u}_{-k}$  and  $\omega_{-k} = -\omega_k$  in the expansion (22). The condition  $u k \ll 1$  has to be held in this method. The solution of Eq. (21) is of the form

$$\vec{u}_k = \frac{e \vec{\mathcal{E}}_k}{2m|\omega_k|} \left( \frac{1}{|\omega_k| + \Omega} + \frac{1}{|\omega_k| - \Omega} \right). \quad (23)$$

According to the quantum mechanical approach, Eq. (23) should be modified as

$$\vec{u}_k = \frac{e \vec{\mathcal{E}}_k}{2m|\omega_k|} \left( \frac{\sqrt{1+n_k}}{|\omega_k| + \Omega} + \frac{\sqrt{n_k}}{|\omega_k| - \Omega} \right), \quad (24)$$

where  $n_k$  is the number of quanta, the first term relates to the quanta emission, and the second one to the absorption.

The mean squared displacement is

$$\langle u^2 \rangle = \int \frac{d^3 R}{V} \langle u^2 \rangle = \sum_k \langle |\vec{u}_k|^2 \rangle, \quad (25)$$

where  $V$  is the volume of the system. Since in our case  $n_k = 0$ , the mean squared displacement has the form

$$\langle u^2 \rangle = \frac{e^2}{4m^2} \sum_k \frac{\langle |\vec{\mathcal{E}}_k|^2 \rangle}{\omega_k^2 (|\omega_k| + \Omega)^2}. \quad (26)$$

The energy of zero point oscillations is

$$\int \frac{d^3R}{4\pi} \langle \mathcal{E}^2 \rangle = \frac{V}{4\pi} \sum_k \langle |\vec{\mathcal{E}}_k|^2 \rangle = \sum_k \frac{\hbar |\omega_k|}{2}. \quad (27)$$

It follows from here that  $\langle |\vec{\mathcal{E}}_k|^2 \rangle = 2\pi\hbar|\omega_k|/V$ . Using the summation rule

$$\sum_k = 2 \int \frac{4\pi k^2 dk V}{(2\pi)^3} \quad (28)$$

(the coefficient 2 accounts for two photon polarizations) and the relation  $\omega_k = ck$ , one can obtain from Eq. (26) [7]

$$\langle u^2 \rangle = \frac{r_B^2}{\pi} \left( \frac{e^2}{\hbar c} \right)^3 \int_0^{\omega_{max}} \frac{\omega d\omega}{(\omega + \Omega)^2}. \quad (29)$$

The upper limit  $\omega_{max}$  is determined by the condition of non-relativistic motion, that is  $\omega_{max} \simeq mc^2/\hbar$ . In the relativistic region  $\vec{u}_k$  decreases due to the enhancement of the relativistic mass. Using the above rydberg estimate for  $\hbar\Omega$  one can obtain for the thread radius

$$r_T = \sqrt{\langle u^2 \rangle} = r_c \sqrt{\frac{2e^2}{\pi\hbar c} \ln \frac{\hbar c}{e^2}}, \quad (30)$$

where  $r_c = \hbar/(mc) \simeq 3.86 \times 10^{-11} \text{cm}$  is the electron Compton length. The exact cut off  $\Omega$  is not crucial for the estimate. The applicability condition of the approach used  $\langle u^2 \rangle k_{max}^2 \sim \langle u^2 \rangle / r_c^2 \ll 1$  is valid since  $\langle u^2 \rangle / r_c^2 \sim e^2/(\hbar c)$ .

## B. Thread properties

When the wave function is smooth one can consider the electron motion in the effective potential  $\langle V(\vec{R} + \vec{u}) \rangle$  averaged on fast electron motions  $\vec{u}$ . Expansion up to the second order in  $\vec{u}$  and using Eq. (30) produces the Lamb shift [7] coincided (excepting the numerical coefficient) with the exact result [6].

When the solution of quantum mechanical equations is singular, it is cut off at the distance  $r_T$ . The thread radius can be estimated from Eq. (30) as  $r_T \simeq 0.15 r_c \simeq 0.58 \times 10^{-11} \text{cm}$ .

At distances  $r_T < r$  radiation effects are small and one can use the quantum mechanical description of the electron. At  $r_c < r$  this is the Schrödinger formalism but at  $r_T < r < r_c$  one should apply Dirac equations. In this case, besides the term  $\ln r$ , the wave function also contains the term  $r_c/r$  which is small at  $r_c \ll r$ . See

Appendix (A.4). The total number of electrons is determined by the region  $r \sim r_B$  outside the thread as in a covalent bond. The fraction of electrons in the region  $r < r_c$  is small as  $r_c^2/r_B^2 \sim (e^2/\hbar c)^3$ .

The wave function is schematically plotted in Fig. 2(a) where it almost corresponds to the quantum mechanical approach (weak radiation corrections) outside the thread. Inside the thread the wave function has the peak which can be interpreted as one resulted from a narrow potential well. Inside the thread the electron state is coupled to the electromagnetic subsystem and cannot be considered separately. Only the total thread energy has a meaning without its separation on electron and electromagnetic ones.

The exact state, where the electron is coupled to photons, is steady and is characterized by the certain total energy which is conserved. In terms of Schrödinger equation it would be an energy eigenvalue. The state, considered either far from the thread or inside it, corresponds to the same energy. The large contribution to the electron kinetic energy  $\sqrt{(mc^2)^2 + (\hbar c/r_T)^2} - mc^2 \simeq 2.93 \text{ MeV}$  inside the thread should be compensated by a reduction of the electromagnetic energy. The latter can be interpreted as a potential well at the thread region in Fig. 2(b) instead of the dashed curve indicating the usual Coulomb potential. One can say that the thread state with the chemical energy scale  $E \sim (1 - 10) \text{ eV}$  corresponds to upper energy states in the deep potential well, of the order of 1 MeV, and of the radius  $r_T$ . This well is extended along the thread.

We emphasize that the interpretation in terms of the potential well is approximate since this is not a single particle quantum mechanics but coupling to the electromagnetic system.

The reduction of the electromagnetic energy reminds the van der Waals phenomenon when the negative potential between atoms is also formed by the reduction of the energy of zero point electromagnetic oscillations [8, 9].

The electron thread energy is continuous and when it is smaller than the lowest level in Fig. 2(b) the thread state can be destroyed by quanta absorption only. The high energy parts, involved into thread formation, correspond to the typical time  $10^{-22} \text{s}$ . Optical processes are slow compared to that time. They lead to an adiabatic motion of the thread parameters but the absorption probability of such quanta is exponentially small [5]. The life time of the thread bond itself is exponentially large (practically infinity) until a high energy particle or  $\gamma$ -quantum destroys it. Also the thread bond cannot be created in chemical or optical processes. The above high energy impact is necessary for that.

The length of the thread bond and a form of the outer electron cloud are determined by chemical mechanisms of interaction with surrounding electrons. The electron density is mainly localized outside the thread on the usual distance of the order of the Bohr radius as in a covalent bond.

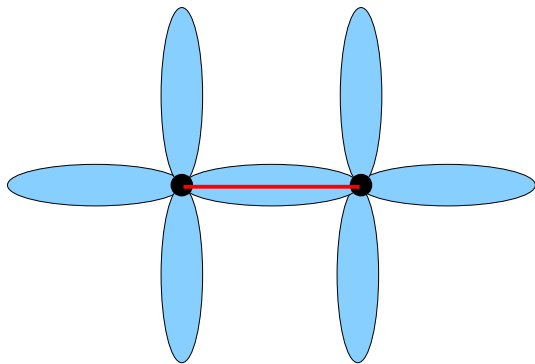


FIG. 3: Schematic representation of molecular covalent bonds. The thread bond between two nuclei is shown by the line.

#### IV. DISCUSSIONS

It looks unusual if energies, involved into molecular bonding, are of the order of 1 MeV and the spatial scale is  $10^{-3}$  of the size of hydrogen atom. At the first sight, it is impossible since chemical bonding is associated with the atomic processes. The point is that the electron state can have a tendency to be singular along the line (thread) connected two nuclei in a molecule. This singularity is cut off by electron interaction with zero point electromagnetic oscillations. The electron also “vibrates” within the thread of the small radius  $r_T$  where the singularity smears out.

The singularity smearing is associated with non-conservation of the electron momentum. The uncertainty of this momentum is  $\hbar/\sqrt{\langle u^2 \rangle}$ . In the absence of external potential, as follows from (29), the mean squared displacement is infinite ( $\Omega = 0$ ). In this case the uncertainty of the electron momentum is zero and the singularity is not cut off. This also follows from the exact spectral representation of the electron Green’s function in the absence of external fields [6].

The peak of electron wave function in the thread region is associated with formation of the certain deep ( $\sim 1$  MeV) potential well along the thread. The potential well is due to the reduction of the energy of electromagnetic zero point oscillations. The interpretation of thread bonding can be in terms of an electron state with the energy  $E \sim (1 - 10)$  eV which corresponds to upper energy states in the deep well. The interpretation in terms of the potential well is approximate since this is not a single particle quantum mechanics but coupling to the electromagnetic system.

This phenomenon is described by quantum electrodynamics since due to short scales the electron momentum becomes relativistic. This is not the unique situation of application of quantum electrodynamics in chemistry. The famous example is van der Waals forces when quantum electrodynamics is involved. In that case also the certain steady attraction potential is formed due to the reduction of the energy of electromagnetic zero point os-

cillations.

Since high energy is involved into the thread formation it cannot be created (or destroyed if it exists) by chemical or optical processes. It can be created by a high energy particle or  $\gamma$ -quantum. After that the thread bond lives the exponentially large (practically infinity) time. A high energy process, of the above type only, can destroy it.

The schematic representation of the thread bond in a molecule is in Fig. 3. The thin thread connects two partner sides. The thread bond is associated with the outer covalent part where the electron cloud is mainly localized (not on the thread).

External high energy radiation (natural or artificial) can result in accumulation of thread bonds in biological molecules, for example in DNA. One can put a question how thread bonds will affect biological processes, for example, replication of DNA.

#### V. CONCLUSIONS

Unusual chemical bonds are proposed. Each bond is almost covalent but is characterized by the thread of a small radius,  $\sim 0.6 \times 10^{-11}$  cm, between two nuclei in a molecule. The main electron density is concentrated outside the thread as in a covalent bond. The thread is formed by the electron wave function which has a tendency to be singular on it. The singularity along the thread is cut off by electron “vibrations” due to the interaction with zero point electromagnetic oscillations. The electron energy has its typical value of  $(1 - 10)$  eV. Due to the small thread radius the uncertainty of the electron momentum inside the thread is large resulting in a large electron kinetic energy  $\sim 1$  MeV. This energy is compensated by formation of a potential well due to the reduction of the energy of electromagnetic zero point oscillations. This is similar to formation of a negative van der Waals potential. Thread bonds are stable and cannot be created or destructed in chemical or optical processes.

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#### Appendix: SINGULAR SOLUTION OF DIRAC EQUATIONS

Schrödinger equation formally has the solution  $\ln r$  in cylindrical coordinates. Below we establish the continuation of this singular solution to the region  $r < r_c$  where one should use the Dirac formalism. In this case the wave function is bispinor consisting of two spinors  $\varphi$  and  $\chi$  [6]. Since we are interested by the singular wave functions (large kinetic energy part) one can ignore potential

energy and consider free electron Dirac equations

$$[E_0 - i\hbar c(\vec{\sigma}\nabla)]\chi = mc^2\varphi, \quad [E_0 + i\hbar c(\vec{\sigma}\nabla)]\varphi = mc^2\chi, \quad (\text{A.1})$$

where  $E_0$  is the total relativistic energy and  $\vec{\sigma}$  are the Pauli matrices [6]. Substituting the spinor  $\chi$  from the second equation (A.1) into the first one we obtain

$$(E_0^2 + \hbar^2 c^2 \nabla^2)\varphi = m^2 c^4 \varphi. \quad (\text{A.2})$$

The equation for  $\chi$  is the same. We use here the relation  $(\vec{\sigma}\nabla)(\vec{\sigma}\nabla) = \nabla^2$ . These equations have solutions  $N_0(r\sqrt{E_0^2/c^2 - m^2 c^2}/\hbar)$  and  $(\vec{\sigma}\nabla)N_0$  where  $N_0$  is the Neuman function [10].

We use the asymptotic forms  $N_0 \sim \ln r$  and  $\nabla N_0 \sim \vec{r}/r^2$ . Those solutions are compatible with the equations

(A.1) if to put

$$\varphi = \varphi_0 \ln r - \frac{ir_c}{2r^2}(\vec{r}\vec{\sigma})\varphi_0, \quad \chi = \varphi_0 \ln r + \frac{ir_c}{2r^2}(\vec{r}\vec{\sigma})\varphi_0, \quad (\text{A.3})$$

where  $\varphi_0$  is some constant spinor. Eqs. (A.3) account for the condition that for our non-relativistic energies  $(E_0 - mc^2) \ll mc^2$ , two spinors should coincide at large distances  $r_c \ll r$  [6]. In the standard representation  $\Phi = \varphi + \chi$  and  $\Theta = \varphi - \chi$

$$\Phi = 2\varphi_0 \ln r, \quad \Theta = -\frac{ir_c}{r^2}(\vec{r}\vec{\sigma})\varphi_0 \quad (\text{A.4})$$

at large distances (non-relativistic limit) the wave function is the usual spinor  $\Phi$ .

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